Study of the one-dimensional Schroedinger equation generated from the hypergeometric equation

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Original English Summary. - A systematic method of constructing potentials, for which the one-variable Schroedinger equation can be solved in terms of the hypergeometric (HGM) function, is presented. All the potentials, obtained by energy-independent transformations of the HGM equation, are determined together with eigenvalues and eigenfunctions. A class of potentials derived from the confluent HGM equation is found by means of a limit process.

To study theoretically the rotational and rotational-vibrational spectra of diatomic molecules, one often uses one-dimensional model potentials for which the solution can be expressed in terms of the HGM functions [1]. The problem of the changes of variable in the HGM equation leading to the one dimensional Schroedinger equation has been studied several times in the past [1, 2, 3], but the quoted authors have considered only the case of potentials given in explicit form [1]. However, knowing the energy spectrum and the wavefunctions of the equation may prove useful for many applied problems whether or not the potential is given in explicit or implicit form.

The general form of the transformations leading from the HGM equation to the Schroedinger equation is determined by the requirement ($z' = dz/dx$)

$$(z')^2 I(z) + \frac{1}{2}\{z, x\} = k^2 - 2MU(x) \ , \tag{1}$$

where

$$I(z) = \frac{(1 - \lambda_0^2)(1 - z) + (1 - \lambda_1^2)z + (\mu^2 - 1)z(1 - z)}{4z^2(1 - z)^2} \ ; \tag{2}$$

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[1]The existence of potentials $U(x)$, not explicitly depending on x, has been first posed in [1] (see also [4]).

and $\{z, x\}$ is the Schwartzian derivative of $z(x)$ with respect to x

$$\{z, x\} = \frac{z''}{z'}\left[\frac{z'''}{z''} - \frac{3}{2}\frac{z''}{z'}\right] ; \tag{3}$$

$U(x)$ is the potential function; M is the reduced mass; $E = \frac{k^2}{2M}$ is the energy. When condition (1) is fulfilled the wavefunction Ψ is related to the HGM function as follows

$$\Psi[z(x)] = (z')^{-1/2} z^{\frac{\lambda_0+1}{2}}(1-z)^{\frac{\lambda_1+1}{2}} F(\alpha, \beta, \gamma; z) . \tag{4}$$

Here

$$\begin{cases} \lambda_0 = \gamma - 1, \\ \lambda_1 = \alpha + \beta - \gamma, \\ \mu = \beta - \alpha. \end{cases} \tag{5}$$

We shall assume that $z(x)$ and therefore also $\{z, x\}$ do not depend on the energy E. In this case, comparing the lhs and rhs of Eq.(1) one concludes that the parameters μ^2, λ_0^2 and λ_1^2 are linear in k^2

$$\begin{cases} 1 - \mu^2 = ak^2 - f \\ 1 - \lambda_p^2 = c_p k^2 - h_p \quad p = 0, 1 \end{cases} \tag{6}$$

and therefore $z(x)$ fulfills the differential equation

$$\frac{(z')^2 R(z)}{4z^2(1-z)^2} = 1 \tag{7}$$

where

$$R(z) = a(z-1)z + c_0(1-z) + c_1 z \tag{8a}$$

or in a slightly different form

$$R(z) = az^2 + b_0 z + c_0 = a(z-1)^2 + b_1(z-1) + c_1 . \tag{8b}$$

Introducing in $\{z, x\}$ the logarithmic derivatives of z' and z'' that can be found using Eq.(7), one next gets the potential from Eq.(1) by means of Eq.(6)

$$2MU[z(x)] = \frac{fz(z-1) + h_0(1-z) + h_1 z + 1}{R} + \left[a + \frac{a + (c_1 - c_0)(2z-1)}{z(z-1)} - \frac{5}{4}\frac{\Delta}{R}\right]\frac{z^2(1-z)^2}{R^2} \tag{9}$$

where the discriminant $\Delta = b_p^2 - 4ac_p = (a - c_1 - c_0)^2 - 4c_1 c_0$.

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Thus, one will get a *semiparametric* (i.e., including the constant of integration of the differential equation) family of potential curves, for one can always choose in the role of the three parameters, the scale factor, the origin of the coordinate x and the origin of the energy E.

For the Schroedinger solution given by Eq.(4) the variable z is considered within the interval $[0,1]$. The corresponding interval for the variable x will be studied shortly.

Since the case of the potential well of infinite depth is not of much interest, we shall ask the three-term quadratic polynomial $R(z)$ to have no zeros for $0 < z < 1$, that is we shall consider

$$R(z) > 0 . \tag{10}$$

It follows from Eq.(7) that in the unit interval the function $z(x)$ is monotone so that the corresponding transformation is single valued. Eq.(10) implies [2]

$$c_p \geq 0 \tag{11a}$$

$$a < (\sqrt{c_1} + \sqrt{c_0})^2 . \tag{11b}$$

Integrating Eq.(7) gives

a) $\Delta \neq 0$

$$\pm 2x = \sum_{p=0}^{1} (-1)^p \left[\sqrt{c_p} \ln |b_p - 2\sqrt{c_p} t_p| - b_p \int \frac{dt_p}{t_p^2 - a} \right] \tag{12a}$$

where $t_p = \frac{\sqrt{r} - \sqrt{c_p}}{z - p}$;

b) $\Delta = 0$

$$\pm 2(x - x_0) = \sum_{p=0}^{1} (-1)^p \sqrt{c_p} \ln |z - p| . \tag{12b}$$

The transformation $z(x)$ can be obtained in explicit form only for a few particular values of the parameters a and c_p. One should notice the case when the zeros of R coincide with the singularities of the HGM equation. The resulting potentials have been already considered by various authors as follows

a) Poeschl-Teller potentials [5] ($R = b_0 z(1 - z)$ or $R = b_0$):

$$2Mb_0 U(x) = \begin{cases} f + 1 - \dfrac{h_0 + \frac{3}{4}}{\sin^2(x/\sqrt{b_0})} - \dfrac{h_1 + \frac{3}{4}}{\cos^2(x/\sqrt{b_0})} & (13a) \\[2ex] h_1 + 1 + \dfrac{h_0 + \frac{3}{4}}{\mathrm{sh}^2(x/\sqrt{b_0})} - \dfrac{f + \frac{3}{4}}{\mathrm{ch}^2(x/\sqrt{b_0})} & (13b) \end{cases}$$

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[2]For $\Delta > 0$, $a > 0$ the coefficients b_0 and b_1 should be of the same sign, i.e., $b_0 b_1 = (c_1 - c_0)^2 - a^2 > 0$.

b) Rosen-Morse potentials [6] $(R = c_0)$

$$2Mc_0 U(x) = \frac{h_0 + h_1 + 2}{2} + \frac{h_0 - h_1}{2} \text{th}(x/\sqrt{c_0}) - \frac{1}{4} \frac{f}{\text{ch}^2(x/\sqrt{c_0})} \tag{14}$$

c) Manning-Rosen potentials [7] $(R = az^2)$

$$2Ma U(x) = \frac{f + h_1 + 2}{2} + \frac{f - h_1}{2} \text{cth}(x/\sqrt{a}) - \frac{1}{4} \frac{h_0}{\text{sh}^2(x/\sqrt{a})} . \tag{15}$$

The potentials (13-15) have the following general properties: the isotopic shift can be described by means of some changes of the parameters f, h_0 and h_1. This property does not extend to the whole family of potential curves given by Eq.(9). The scale transformation of the coordinate x leads in this case to an equation with five singular points, 0, 1, z_1, z_2, and ∞, where z_1 and z_2 are the zeros of R.

Let us find now the interval where x is defined for $\Delta \neq 0$. For that, we first notice that the integral entering Eq. (12a) has no singularities, because from $t_p = \sqrt{a}$ or

$$\sqrt{a + \frac{b_p}{z - p} + \frac{c_p}{(z - p)^2}} = \sqrt{a} + \frac{c_p}{z - p}$$

$\Delta = 0$ would follow. This is why, performing $z \to p$ $(t_p \to b_p/2\sqrt{c_p})$ in Eq. (12), we get the limits $\pm\infty$ in x for $c_p \neq 0$; if however one of the coefficients c_p is nought then the corresponding choice of the coordinate origin for x as well as of the sign in Eq.(12a) can be done such that

$$0 \leq x < \infty .$$

Finally, the variable x has a finite definition interval whenever both c_0 and c_1 are zero.

The case when only one of the c_p coefficients, for example c_0, is zero, is of special interest for the theory of two atom molecules, because for $x \to 0$ $(z \to 0)$ the function $2Mb_0 U(x)$ goes to infinity as $(h_0 + \frac{3}{4})z^{-1}$. For this potential, contrary to the Morse case, the Schroedinger equation is solved with regular boundary conditions for $x = 0$ (see [8]).

If $h_0 = \frac{3}{4}$, the potential $U(x)$ is finite at the origin and for $x \geq 0$ $(0 \leq z \leq 1)$ reads

$$2Ma U[z(x)] = \frac{f(z - 1) + h_1 + \frac{3}{4}}{z - z_1} + 1 + \frac{3}{4} \frac{(3z_1 - 1)(1 - z_1)}{(z - z_1)^2} - \frac{5}{4} \frac{z_1(1 - z_1)^2}{(z - z_1)^3} \tag{16}$$

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For $x < 0$ it is natural to a priori determine the potential Eq.(16) to be symmetric $U(x) = U(-x)$.

Notice that for

$$-\frac{1}{4} - \frac{9}{4}\frac{(1 - z_1)}{z_1} > (f + \frac{3}{4})(1 - z_1) > -1$$

the potential Eq.(16) has two symmetric minima separated by a small barrier.

Since the HGM solution which is irregular at $z = 1$ has a $(1 - z)^{-\lambda_1}$ $(\lambda_1 > 0)$ behavior at that point, the integral

$$\int_0^\infty \Psi^2 dx = \frac{1}{4} \int_0^1 R z^{\lambda_0 - 1}(1 - z)^{\lambda_1 - 1}[F(\alpha, \beta, \gamma; z)]^2 dz \tag{17}$$

is finite only if α (or β) is equal either to a negative integer or zero: $\alpha = -n$. The eigenfunctions $\Psi_n^\pm$ are determined by the conditions

$$\frac{d\Psi_n^+}{dx}|_{x=0} = 0 \tag{18a}$$

and

$$\Psi_n^-(0) = 0 , \tag{18b}$$

leading to a finite integral Eq. (17). The energy spectrum is determined by

$$p + \frac{1}{2} + \sqrt{h_1 + 1 - c_1 k_p^2} = \sqrt{f + 1 - a k_p^2} , \tag{19}$$

where $p = 2n$ for even levels and $p = 2n + 1$ for the odd ones, respectively.

Let us clarify now under what conditions the potential Eq.(9) leads to a discrete spectrum. We shall consider $c_1 \neq 0$. For a discrete spectrum to occur, the function $(z')^{-\frac{1}{2}}\Psi$ should go to ∞ when $z \to 0$ at least as $z^{-\frac{1}{2}}$, if one takes Ψ as the general solution of the Schroedinger equation. This condition is obviously true for $c_0 \neq 0$. If $c_0 = 0$ the existence of the discrete spectrum is possible only for positive values of h_0. The energy levels come from the equation

$$2n + 1 = \sqrt{f + 1 - a k_n^2} - \sqrt{h_0 + 1 - c_0 k_n^2} - \sqrt{h_1 + 1 - c_1 k_n^2} . \tag{20}$$

It is easy to see that the spectrum is bounded from above, if and only if both c_0 and c_1 are not zero, and therefore, it follows from Eq.(20) that the discrete part of the spectrum has only a finite set of energy levels. Only the potential curve Eq.(13a), for which $c_0 = c_1 = 0$, has an infinity of discrete levels.

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The eigenfunctions of the discrete spectrum are of the form

$$\Psi_n = B_n z^{\frac{\lambda_0-1}{2}}(1-z)^{\frac{\lambda_1-1}{2}}(Rz')^{\frac{1}{2}} P_n^{(\lambda_1,\lambda_2)}(2z-1) \ . \tag{21}$$

Here $P_n^{(\lambda_1,\lambda_0)}(2z-1)$ are the Jacobi polynomials, whereas B_n is a normalization constant given by

$$B_n = \left[\left(\frac{c_1}{\lambda_1} + \frac{c_0}{\lambda_0} - \frac{a}{\mu} \right) \frac{\Gamma(\lambda_0+n+1)\Gamma(\lambda_1+n+1)}{n!\Gamma(\mu-n)} \right]^{-\frac{1}{2}} , \tag{22}$$

(see the integrals 7.391 (1) and (5) in [9]). In particular, the eigenfunctions $\Psi_n^{(\pm)}$, corresponding to the potential Eq.(16), are obtained from Eq. (21) for $c_0 = 0, \lambda_0 = \pm\frac{1}{2}$.

We notice that the potential curve Eq.(13a) displays one more important property: the Jacobi polynomials for neighbour energy levels are connected by simple recurrence relationships (the parameters λ_0 and λ_1 does not depend in this case on energy), and the matrix elements $\langle m|z|n \rangle$ is different from zero for $m = n, n \pm 1$.

To pass to the limit of the confluent HGM equation we make the following notations

$$a = \frac{\sigma_2}{\tau^2}, \quad c_1 = \frac{\sigma_2}{\tau^2} + \frac{\sigma_1}{\tau} + c_0 \qquad (b_0 = \frac{\sigma_1}{\tau}), \tag{23a}$$

$$f = \frac{g_2}{\tau^2}, \quad h_1 = \frac{g_2}{\tau^2} + \frac{g_1}{\tau} + h_0 \tag{23b}$$

and

$$z = \tau\zeta \ . \tag{24}$$

For $\tau \to 0$ we have

$$\frac{(\zeta')^2 R(\zeta)}{4\zeta^2} = 1 \ , \tag{25}$$

$$I(\zeta) = -\frac{\delta_2}{4} - \frac{\delta_1}{4\zeta} + \frac{1-\lambda_0^2}{4\zeta^2} \ , \tag{26}$$

where

$$\delta_1 = \lim_{\tau\to 0}[\tau(\lambda_1^2 - \mu^2)] = g_1 - \sigma_1 k^2 \ , \tag{27a}$$

$$\delta_2 = \lim_{\tau\to 0}[\tau^2\mu^2] = g_2 - \sigma_2 k^2 \geq 0 \ . \tag{27b}$$

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For $\delta_2 > 0$ [3] the wavefunction Ψ is connected with the Whittaker and the confluent series as follows

$$\Psi = (\zeta')^{-1/2} M_{-\frac{\delta_1}{4\sqrt{\delta_0}}, \frac{\lambda_0}{2}}(\sqrt{\delta_2}\zeta) \tag{28a}$$

or

$$\Psi = (\zeta')^{-1/2}(\sqrt{\delta_2}\zeta)^{\frac{\lambda_0+1}{2}} e^{-\sqrt{\delta_2}\zeta/2} F(\frac{\gamma}{2} + \frac{\delta_1}{4\sqrt{\delta_2}}, \gamma; \sqrt{\delta_2}\zeta) . \tag{28b}$$

The series terminates if

$$-\frac{\gamma}{2} - \frac{\delta_1}{4\sqrt{\delta_2}} = n, \qquad n = 0, 1, 2... \tag{29}$$

The potential $U[\zeta(x)]$ takes the form

$$2MU[\zeta(x)] = \frac{g_2\zeta^2 + g_1\zeta + h_0 + 1}{R} + \left[\frac{\sigma_1}{\zeta} - \sigma_2 - \frac{5\Delta}{4R}\right]\frac{\zeta^2}{R^2} , \tag{30}$$

where $\Delta = \sigma_1^2 - 4\sigma_2 c_0$; here the function $\zeta(x)$ is given in the following implicit form

$$\pm 2(x - x_0) = \sqrt{R} + \sqrt{c_0}\ln|\sigma_1 - 2t\sqrt{c_0}| + \frac{\sigma_1}{2\sqrt{\sigma_2}}\ln|\frac{t + \sqrt{\sigma_2}}{t - \sqrt{\sigma_2}}| , \tag{31}$$

where $t = \frac{\sqrt{R} - \sqrt{c_0}}{\zeta}$.

It is supposed that $R(\zeta)$ has no zeros within $(0, \infty)$, that is

$$\sigma_2 \geq 0, \qquad c_0 \geq 0, \qquad \sigma_1 > -2\sqrt{c_0\sigma_2} . \tag{32}$$

If two of the three parameters σ_1, σ_2 and c_0 turn to zero, Eq.(31) is easy to solve with respect to ζ and the potential leads in this case to: a) a spherically symmetric oscillator well (or barrier) for $\sigma_2 = c_0 = 0$ [11]; b) a Morse potential for $\sigma_1 = \sigma_2 = 0$ [12]; a Kratzer potential for $\sigma_1 = c_0 = 0$ [13, 14].

We remark that in the work [15] an implicit potential occurs for which the Schroedinger equation is turned into a confluent HGM equation. This potential can be obtained from Eq.(30), if $\sigma_2 = 0$. The assumptions in [15] may be considered equivalent to a transformation $\zeta(x)$ not depending on energy and therefore the results of [15] can be easily obtained in our framework.

Let us study now the definition interval of x. For $\zeta \to \infty$ x goes to $\pm\infty$ as $\pm\frac{1}{2}\sqrt{\sigma_2}\zeta$, if $\sigma_2 \neq 0$, and as $\pm\sqrt{\sigma_1\zeta}$, if $\sigma_2 = 0$, $\sigma_1 \neq 0$, because in the latter case

$$\pm 2(x - x_0) = \sqrt{R} + \frac{\sigma_1}{t} + \sqrt{c_0}\ln|\zeta t^2| \tag{33}$$

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[3]For $\delta_2 = 0$, $\Psi = (\zeta')^{-1/2}\zeta^{1/2}Z_{\frac{\lambda_0}{2}}(\sqrt{-\delta_1}\zeta^{1/2})$ (see the formula 2, 162 (1a) in [10])

(for $\sigma_2 = 0$, $\sigma_1 = 0$ x varies from $-\infty$ to $+\infty$). For $\zeta \to 0$, $x \to \mp\infty$ if $c_0 \neq 0$, and $x \to x_0$ if $c_0 = 0$.

For $\sigma_2 \neq 0$, the zero of the energy is determined by the condition $U(\infty) = 0$, i.e., $g_2 = 0$. In this case, one gets for the energy spectrum the following equation

$$2n + 1 = -\frac{\sigma_1}{2\sqrt{\sigma_2}}|k_n| - \frac{g_1}{2\sqrt{\sigma_2}|k_n|} - \sqrt{h_0 + 1 - c_0 k_n^2} \ . \tag{34}$$

From this, it follows that

a) for $g_1 \geq 0$, $h_0 + 1 \geq 0$, there is no discrete spectrum, because

$$-\frac{\sigma_1}{2\sqrt{\sigma_2}}|k_n| - \sqrt{h_0 + 1 - c_0 k_n^2} \leq \left[\frac{-\sigma_1}{2\sqrt{\sigma_2}} - \sqrt{c_0}\right]|k_n| \leq 0 \ ; \tag{35}$$

b) for $g_1 \geq 0$, $h_0 + 1 < 0$, a finite number of discrete levels is possible if $\sigma_1 < 0$;

c) for $g_1 < 0$ the discrete spectrum has an infinite number of levels converging to zero. For $\sigma_2 = 0$ the discrete levels are determined by the equation

$$1 + h_0 - c_0 k_n^2 = \left(2n + 1 + \frac{g_1 - \sigma_1 k_n^2}{2\sqrt{g_2}}\right)^2 \tag{36}$$

and for $c_0 \neq 0$ the discrete spectrum may have only a finite number of energy levels (the case $\sigma_2 = 0$, $c_0 = 0$ corresponds to an infinite number of levels).

The wavefunctions of the discrete spectrum are given in terms of the Laguerre polynomials as follows

$$\Psi_n = B_n R^{\frac{1}{2}} (\sqrt{\delta_2}\zeta)^{\frac{\lambda_0 - 1}{2}} e^{-\sqrt{\delta_2}\frac{\zeta}{2}} (\sqrt{\delta_2}\zeta')^{\frac{1}{2}} L_n^{(\lambda_0)} (\sqrt{\delta_2}\zeta) \ . \tag{37}$$

Here, the normalization factor B_n reads

$$B_n = \left[\left(\frac{c_0}{\lambda_0} + \frac{\sigma_1}{\sqrt{\delta_2}} + (\lambda_0 + 2n + 1)\frac{\sigma_2}{\delta_2}\right)\frac{\Gamma(\gamma + n)}{n!}\right]^{-\frac{1}{2}} \ . \tag{38}$$

The integrals required for its calculation can be obtained from I_ν [16]:

$$I_\nu = \int e^{-\sqrt{\delta_2}\zeta} \zeta^{\nu-1} [F(-n, \gamma; \sqrt{\delta_2}\zeta)]^2 d\zeta \tag{39}$$

for $\nu = \gamma \pm 1, \gamma$.

The potentials given by Eqs. (9) and (30) may have useful applications in the theory of diatomic molecules, in particular, for the calculations of important quantities such as the Franck-Condon factors and anharmonic constants.

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